

Cyclophosphamide
50-18-0 | DTXSID5020364

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 1.14 | 0.85 | 1.12 | 0.83 | 1.23 |

Model Results

Predicted value: 2.41×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.73×10^{-1}

Confidence level: 7.23×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Cycloate

Measured: 3.54×10^{-11}

Predicted: 2.98×10^{-11}

Image not found

EPTC

Measured: 3.18×10^{-11}

Predicted: 2.83×10^{-11}

Image not found

Terbutylazine

Measured: 1.10×10^{-11}

Predicted: 1.23×10^{-11}

Image not found

Simazine

Measured: 1.10×10^{-11}

Predicted: 1.22×10^{-11}

Image not found

Triethyl phosphate

Measured: 5.53×10^{-11}

Predicted: 4.26×10^{-11}